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TERMINAL (ENTER 1, 2, 3, OR ?):2
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                Zentralblatt
NEWS 3 OCT 19 BEILSTEIN updated with new compounds
NEWS 4 NOV 15 Derwent Indian patent publication number format enhanced
NEWS 5 NOV 19 WPIX enhanced with XML display format
NEWS 6 NOV 30 ICSD reloaded with enhancements
NEWS 7 DEC 04 LINPADOCDB now available on STN
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NEWS 9 DEC 17 USPATOLD added to additional database clusters
NEWS 10 DEC 17 IMSDRUGCONF removed from database clusters and STN
NEWS 11 DEC 17 DGENE now includes more than 10 million sequences
NEWS 12 DEC 17 TOXCENTER enhanced with 2008 MeSH vocabulary in
                MEDLINE segment
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NEWS 15 DEC 17 STN Viewer enhanced with full-text patent content
                from USPATOLD
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NEWS 17 JAN 16 CAS patent coverage enhanced to include exemplified
                prophetic substances
NEWS 18 JAN 28 USPATFULL, USPAT2, and USPATOLD enhanced with new
                custom IPC display formats
NEWS 19 JAN 28 MARPAT searching enhanced
NEWS 20 JAN 28 USGENE now provides USPTO sequence data within 3 days
                of publication
NEWS 21 JAN 28 TOXCENTER enhanced with reloaded MEDLINE segment
NEWS 22 JAN 28 MEDLINE and LMEDLINE reloaded with enhancements
NEWS 23 FEB 08 STN Express, Version 8.3, now available
NEWS 24 FEB 20 PCI now available as a replacement to DPCI
NEWS 25 FEB 25 IFIREF reloaded with enhancements
NEWS 26 FEB 25 IMSPRODUCT reloaded with enhancements
NEWS 27 FEB 29 WPINDEX/WPIDS/WPIX enhanced with ECLA and current
                U.S. National Patent Classification
NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3.
            AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008
```

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=> file eg 'EG' IS NOT A VALID FILE NAME

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Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files that are available. If you have requested multiple files, you can specify a corrected file name or you can enter "IGNORE" to continue accessing the remaining file names entered.

=> file reg COST IN U.S. DOLLARS FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

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http://www.cas.org/support/stngen/stndoc/properties.html

=>

Uploading C:\Program Files\Stnexp\Queries\10576194.str

```
23 24 25 26 28 29
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22
chain bonds :
1-23 8-17 11-25 14-24 19-23 19-28 21-29 24-29 25-26
ring bonds :
1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11 12-13 12-17 13-14 14-
1.5
15-16 16-17 18-19 18-22 19-20 20-21 21-22
exact/norm bonds :
1-2 \quad 1-5 \quad 1-23 \quad 2-3 \quad 3-4 \quad 4-5 \quad 6-7 \quad 6-11 \quad 7-8 \quad 8-9 \quad 8-17 \quad 9-10 \quad 10-11 \quad 11-25 \quad 14-24
18-19 18-22 19-20 19-23 19-28 20-21 21-22 21-29 24-29 25-26
normalized bonds :
12-13 12-17 13-14 14-15 15-16 16-17
isolated ring systems :
containing 1 : 6 : 12 : 18 :
```

## G1:C, N

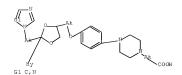
### Match level :

chain nodes :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 23:CLASS 24:CLASS 25:CLASS 26:CLASS 28:Atom 29:CLASS

## L1 STRUCTURE UPLOADED

=> d 11 L1 HAS NO ANSWERS L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11 full

FULL SEARCH INITIATED 18:08:51 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 159 TO ITERATE

100.0% PROCESSED 159 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

L2 0 SEA SSS FUL L1

=> file reg

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 180.66 180.87

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STRUCTURE FILE UPDATES: 6 MAR 2008 HIGHEST RN 1006950-27-1
DICTIONARY FILE UPDATES: 6 MAR 2008 HIGHEST RN 1006950-27-1

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when conducting  ${\tt SmartSELECT}$  searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

= :

Uploading C:\Program Files\Stnexp\Oueries\10576194claim1.str

```
chain nodes :
23 24 26 27 37 40 41 43
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 29
30 31 32 33 34
ring/chain nodes :
35 36 38
chain bonds :
1-23 8-17 11-31 14-24 19-23 19-26 21-27 24-27 34-35 35-36 35-43 36-37
36-38 38-40 38-41
ring bonds :
1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11 12-13 12-17 13-14 14-
15
15-16 16-17 18-19 18-22 19-20 20-21 21-22 29-30 29-34 30-31 31-32 32-33
33-34
exact/norm bonds :
1-2 1-5 1-23 2-3 3-4 4-5 6-7 6-11 7-8 8-9 8-17 9-10 10-11 11-31 14-24
18-19 18-22 19-20 19-23 19-26 20-21 21-22 21-27 24-27 34-35 35-36 35-43
36-37 36-38
38-40 38-41
normalized bonds :
12-13 12-17 13-14 14-15 15-16 16-17 29-30 29-34 30-31 31-32 32-33 33-34
isolated ring systems :
containing 1 : 6 : 12 : 18 : 29 :
```

G1:C, N

G2:C, H

Match level: 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 21:Atom 23:Atom 21:Atom 23:Atom 23

22:Atom 23:CLASS 24:CLASS 26:Atom 27:CLASS 29:Atom 30:CLASS 31:Atom 32:Atom 33:Atom 34:Atom

L3 STRUCTURE UPLOADED

=> d 13

L3 HAS NO ANSWERS

L3 STR

G1 C,N G2 C,H

Structure attributes must be viewed using STN Express query preparation.

=> s 13 full

FULL SEARCH INITIATED 18:12:42 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 57 TO ITERATE

100.0% PROCESSED 57 ITERATIONS SEARCH TIME: 00.00.01 0 ANSWERS

L4 0 SEA SSS FUL L3

Uploading C:\Program Files\Stnexp\Queries\10576194noB.str

```
23 24 26 27
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22
chain bonds :
1-23 8-17 14-24 19-23 19-26 21-27 24-27
ring bonds :
1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11 12-13 12-17 13-14 14-
15-16 16-17 18-19 18-22 19-20 20-21 21-22
exact/norm bonds :
1-2 1-5 1-23 2-3 3-4 4-5 6-7 6-11 7-8 8-9 8-17 9-10 10-11 14-24 18-19
18-22 19-20 19-23 19-26 20-21 21-22 21-27 24-27
normalized bonds :
12-13 12-17 13-14 14-15 15-16 16-17
isolated ring systems :
containing 1 : 6 : 12 : 18 :
```

G1:C,N

G2:C,H

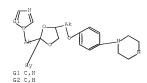
```
Match level :
```

chain nodes :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:CLASS 24:CLASS 26:Atom 27:CLASS

#### L5 STRUCTURE UPLOADED

=> d 15 L5 HAS NO ANSWERS L5 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 15 full FULL SEARCH INITIATED 18:16:06 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 2304 TO ITERATE

100.0% PROCESSED 2304 ITERATIONS SEARCH TIME: 00.00.01 12 ANSWERS

L6 12 SEA SSS FUL L5

=> file caplus COST IN U.S. DOLLARS

 COST IN U.S. DOLLARS
 SINCE FILE
 TOTAL

 ENTRY
 SESSION

 FULL ESTIMATED COST
 359.02
 539.89

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=> s 16 full

L7 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2006:598868 CAPLUS Full-text

DOCUMENT NUMBER: 145:180204

TITLE: Novel ketoconazole analogues based on the replacement of 2,4-dichlorophenyl group with 1,4-benzothiazine

moiety: Design, synthesis, and microbiological

evaluation

AUTHOR(S): Schiaffella, Fausto; Macchiarulo, Antonio; Milanese,

Lara; Vecchiarelli, Anna; Fringuelli, Renata CORPORATE SOURCE: Department of Drug Chemistry and Technology,

University of Perugia, Perugia, 06100, Italy SOURCE: Bioorganic & Medicinal Chemistry (2006), 14(15),

5196-5203 CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 145:180204

AB As a part of a program to develop novel antifungal agents, new compds. which incorporate the 1,4-benzothiazine moiety into the structure of ketoconazole (KTZ) were prepared These compds. were computationally investigated to assess whether the 1,4-benzothiazine moiety was a suitable bioisosteric replacement for the 2,4-dichlorophenyl group of KTZ in order to obtain a more potent inhibition of CYP51 enzyme of Candida albicans. Results of preliminary microbiol. studies show that the racemic cis-7 analog has a good in vivo activity, comparable to that of KTZ, but the best activity was observed in the racemic trans-7 analog.

IT 902799-20-6P 902799-21-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(benzothiazine ketoconazole analogs as antifungal agents)

RN 902799-20-6 CAPLUS

CN Piperazine, 1-acety1-4-[4-[{(2R,4\$)-2-(3,4-dihydro-4-methy1-3-oxo-2H-1,4-benzothiazin-7-y1)-2-(1H-imidazol-1-ylmethy1)-1,3-dioxolan-4-y1]methoxy[pheny1]-, rel- (9C1) (CA INDEX NAME)

Relative stereochemistry.

RN 902799-21-7 CAPLUS

CN Piperazine, 1-acety1-4-[4-[(2R,4R)-2-(3,4-dihydro-4-methy1-3-oxo-2H-1,4-benzothiazin-7-y1)-2-(1H-imidazol-1-y1methy1)-1,3-dioxolan-4-

Relative stereochemistry.

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2005:395302 CAPLUS Full-text

DOCUMENT NUMBER: 142:447236

TITLE: Preparation of 2-(azolylmethyl)-4-

(piperazinylphenoxymethyl)-1,3-dioxolanes as

antifungals with reduced interaction with metabolic

cytochromes.

INVENTOR(S): Pinori, Massimo; Lattanzio, Maria; Modena, Daniela;

Mascagni, Paolo

PATENT ASSIGNEE(S): Italfarmaco S.p.A., Italy

SOURCE: PCT Int. Appl., 27 pp.

CODEN: PIXXD2 Patent

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.					KIND				APPLICATION NO.						DATE			
				A1	_	20050506		WO 2004-EP11667					20041014					
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		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,	
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	
		ΤJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW	
	RW:	BW,	GH,	GM,	KΕ,	LS,	MW,	ΜZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	
		AZ,	BY,	KG,	KZ,	MD,	RU,	ТJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	
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		SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	
		SN,	TD,	TG														
CA				A1				CA 2004-2542361										
EP	1673368				A1	A1 20060628				EP 2004-790506						20041014		
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		IE,	SI,	FΙ,	RO,	CY,	TR,	BG,	CZ,	EE,	HU,	PL,	SK					
								CN 2004-80030607										
BR										BR 2004-15319								
JP	2007533638			T		2007	1122		JP 2006-534715					20041014				

IN 2006DN01807 A 20070810 IN 2006-DN1807 20060403 US 2007129376 A1 20070607 US 2006-576194 20060417 PRIORITY APPLN. INFO.: IT 2003-MI2020 A 20031017 W0 2004-EP11667 W 20041014

OTHER SOURCE(S): CASREACT 142:447236; MARPAT 142:447236

GI

AB Title compds. [I, A = N, CH; Het = heteroaryl optionally substituted by ≥1 5-6 membered aromatic rings; B = alkanoate, 4-C6H4NR2CONRIR3; R1 = H, (substituted) alkyl; R2, R3 = H, alkyl; R2R3 = CH:N, CH:CH, CH2CH2], were prepared Thus, 2,4-dihydro-4-[4-[4-(4-hydroxyphenyl)-1- piperazinyl]phenyl]-2-(1-methyl)proyl)-3H-1,2,4-triazol-3-one in DMF was treated with KOCMe3 and then with cis-[2-(pyridin-2-yl)-2-(1,2,4-triazol-1- ylmethyl)-1,3-dioxolan-4-ylmethyl) tosylate in DMF followed by heating at 130° for 3 h to give 28 cis-4-[4-[4-[4-(2-(pyridin-2-yl)-2-(1H-1,2,4-triazol-1-ylmethyl)-1,3-dioxolan-4-ylmethoxy]phenyl]-1- piperazinyl]phenyl]-2-(1-methoxypropyl)-2,4-dihydro-3H-1,2,4-triazol-3- one. The latter at 50 mg/kg/day in mice infected with Candida albicans gave a mean survival time of 9.1 days, vs. 5.3 for untreated controls.

IT 851341-62-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(claimed compound; preparation of

azolvlmethylpiperazinylphenoxymethyldioxolan

es as antifungals with reduced interaction with metabolic cytochromes)

RN 851341-62-3 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 2,4-dihydro-2-(1-methylpropy1)-4-[4-[4-[4-[4-[4-R-2]] (2R,4R)-2-(2-pyridiny1)-2-(1H-1,2,4-triazol-1-ylmethy1)-1,3-dioxolan-4-yllmethoxylphenyl]-1-piperazinyllphenyl]-, rel (CA INDEX NAME)

Relative stereochemistry.

IT 851341-72-5P 851341-73-6P 851341-74-7P 851341-75-8P 851341-76-9P 851341-77-0P 851341-78-1P 851341-79-2P 851341-80-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of azolylmethylpiperazinylphenoxymethyldioxolanes as antifungals with reduced interaction with metabolic cytochromes)

RN 851341-72-5 CAPLUS

CN 3H-1, 2, 4-Triazol-3-one, 2, 4-dihydro-2-(1-methylpropyl)-4-[4-[4-[4-[(2R,4S)-2-(4-pyridinyl)-2-(1H-1,2,4-triazol-1-ylmethyl)-1,3-dioxolan-4-yl]methoxylphenyl]-1-piperazinyllphenyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

RN 851341-73-6 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 2,4-dihydro-2-(1-methylpropyl)-4-[4-[4-[4-[(2R,4S)-2-(3-pyridinyl)-2-(1H-1,2,4-triazol-1-ylmethyl)-1,3-dioxolan-4-yl]methoxylphenyl]-1-piperazinyllphenyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

RN 851341-74-7 CAPLUS

CN 3H-1, 2, 4-Triazol-3-one, 2, 4-dihydro-2-(1-methylpropyl)-4-[4-[4-[4-[(2R,4R)-2-(2-thiazolyl)-2-(1H-1,2,4-triazol-1-ylmethyl)-1,3-dioxolan-4-yl]methoxylphenyl]-1-piperazinyllphenyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

RN 851341-75-8 CAPLUS

CN 3H-1, 2, 4-Triazol-3-one, 2, 4-dihydro-2-[(1S)-1-methylpropyl)-4-[4-[4-[4-[4-[(2R,4R)-2-(2-pyridinyl)-2-(1H-1,2,4-triazol-1-ylmethyl)-1,3-dioxolan-4-yl]methoxylphenyl]-1-piperazinyllphenyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 851341-76-9 CAPLUS

Absolute stereochemistry.

RN 851341-77-0 CAPLUS

CN 3H-1, 2, 4-Triazol-3-one, 2, 4-dihydro-2-[(1R)-1-methylpropyl]-4-[4-[4-[4-[(2R,4R)-2-(2-pyridinyl)-2-(1H-1, 2, 4-triazol-1-ylmethyl)-1, 3-dioxolan-4-yl]methoxylphenyl]-1-piperazinyllphenyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 851341-78-1 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 2,4-dihydro-2-[(1R)-1-methylpropyl]-4-[4-[4-[4-[4-[(2S,4S)-2-(2-pyridinyl)-2-(1H-1,2,4-triazol-1-ylmethyl)-1,3-dioxolan-4-ylmethoxylphenyl]-1-piperazinyllphenyl]- (CA INDEX NAME)

Absolute stereochemistry.

RN 851341-79-2 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 2,4-dihydro-2-(1-methylpropyl)-4-[4-[4-[4-[[(2R,4R)-2-(1-oxido-2-pyridinyl)-2-(1H-1,2,4-triazol-1-ylmethyl)-1,3dioxolan-4-yl]methoxy]phenyl]-1-piperazinyl]phenyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

RN 851341-80-5 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 2,4-dihydro-2-(1-methylpropyl)-4-[4-[4-[4-[(2R,45)-2-(1-oxido-4-pyridinyl)-2-(1H-1,2,4-triazol-1-ylmethyl)-1,3dioxolan-4-yl]methoxy]phenyl]-1-piperazinyl]phenyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

PAGE 1-B



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 18:08:15 ON 07 MAR 2008)

FILE 'REGISTRY' ENTERED AT 18:08:25 ON 07 MAR 2008 L1 STRUCTURE UPLOADED

L2 0 S L1 FULL

FILE 'REGISTRY' ENTERED AT 18:12:15 ON 07 MAR 2008

L3 STRUCTURE UPLOADED

L4 0 S L3 FULL

L5 STRUCTURE UPLOADED

L6 12 S L5 FULL

FILE 'CAPLUS' ENTERED AT 18:16:13 ON 07 MAR 2008

L7 2 S L6 FULL

=> log y
COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 16.66 556.55

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL
ENTRY SESSION
ENTRY SESSION
ENTRY SESSION
ENTRY SESSION

CA SUBSCRIBER PRICE -1.60 -1.60

STN INTERNATIONAL LOGOFF AT 18:23:30 ON 07 MAR 2008